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Studies of soot formation in turbulent jet flames burning ethylene in air were studied for Reynolds numbers ranging from 4000 to 23,000. Laser-based techniques were used to measure the soot volume fraction, particle size and number density as well as the temperature and relative concentration of hydroxyl radicals and polycyclic aromatic hydrocarbons. Measurements of the characteristics length scales for the soot and hydroxyl radical fields throughout the turbulent flames were obtained. The maximum soot eddy size was observed to be 7 mm or about three times the size of the diameter of the fuel jet (d= 2.18 mm). The soot eddy size increased linearly along the centerline of the turbulent flame until the mid-point, where it leveled off and finally decreased in the oxidation zone. In contrast, the hydroxyl radical eddy size always increased along the flame with a maximum eddy size of 12 mm for the higher Reynolds number flames. Analysis of the radial dependence of the eddy size was also determined. Relatively little radial dependence in the eddy size was observed for the soot particles indicating that the soot eddies moved off the axis very fast as compared to the mixing rate. However for the hydroxyl radicals, the eddy size was always larger off the axis of the flame except near the flame tip. With respect to the temperature field, temperature probability density functions indicated bimodality at all axially locations. With respect to soot formation, the highest soot formation location and the peak mean temperature were observed on the fuel-rich side of the stoichiometric flame location while the peak hydroxyl radical concentration was on the fuel-lean side.

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Progress Report 1998

Soot Formation in Turbulent Combusting Flows

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Studies of soot formation in turbulent jet flames burning ethylene in air were studied for Reynolds numbers ranging from 4000 to 23,000. Laser-based techniques were used to measure the soot volume fraction, particle size and number density as well as the temperature and relative concentration of hydroxyl radicals and polycyclic aromatic hydrocarbons. Measurements of the characteristics length scales for the soot and hydroxyl radical fields throughout the turbulent flames were obtained. The maximum soot eddy size was observed to be 7 mm or about three times the size of the diameter of the fuel jet (d= 2.18 mm). The soot eddy size increased linearly along the centerline of the turbulent flame until the mid-point, where it leveled off and finally decreased in the oxidation zone. In contrast, the hydroxyl radical eddy size always increased along the flame with a maximum eddy size of 12 mm for the higher Reynolds number flames. Analysis of the radial dependence of the eddy size was also determined. Relatively little radial dependence in the eddy size was observed for the soot particles indicating that the soot eddies moved off the axis very fast as compared to the mixing rate. However for the hydroxyl radicals, the eddy size was always larger off the axis of the flame except near the flame tip. With respect to the temperature field, temperature probability density functions indicated bimodality at all axially locations. With respect to soot formation, the highest soot formation location and the peak mean temperature were observed on the fuel-rich side of the stoichiometric flame location while the peak hydroxyl radical concentration was on the fuel-lean side.

SOOT FORMATION IN TURBULENT COMBUSTING FLOWS

(AFOSR Grant/Contract No. F49620-97-1-0094)

Principal Investigator: R. J. Santoro

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SUMMARY/OVERVIEW

Current interest in high performance, low emissions gas turbine engines by the Air Force underscores the need for research on soot formation processes, since soot formation is directly related to issues involving performance and operability. Although recent research has provided significant advances in terms of understanding the basic mechanism controlling soot formation and destruction, many questions remain. In particular, an understanding of soot formation under high pressure and turbulent flame conditions is lacking. Since gas turbine combustors characteristically involve such flows, it is necessary to address these conditions if further progress is to be made. The current study is specifically directed at providing measurements of soot formation and destruction in atmospheric and high pressure turbulent flames. To date, measurements of the soot volume fraction, temperature and relative OH radical concentrations have been obtained for atmospheric flames over a Reynolds number range of 4000 to 23,000 for ethylene jet flames. These measurements have yielded quantitative information of the quantity of soot formed, the probability density functions for soot volume fraction, relative OH radical concentration, and temperature as well as providing determinations of the evolution of the integral length scales in the flame as a function of flame position and Reynolds number. This data is intended to form the basis for validating models of flame systems representative of gas turbine combustors. Such modeling capability is required to develop the needed insight necessary for implementing advanced design methodologies for future gas turbine combustors.

TECHNICAL DISCUSSION

Studies of soot formation in turbulent diffusion flames under atmospheric and elevated pressure conditions are being conducted to determine the controlling phenomena governing soot inception, growth and oxidation. Ethylene (C_2H_4) has been selected as the fuel and the soot formation process in the turbulent diffusion flames resulting from combustion of the fuel jet issuing into quiescent air is being investigated as a function of Reynolds number. Fuel jets issuing from tubes of 2.18 and 4.12 mm have been studied for Reynolds numbers ranging from 4000 to 23,000. The flame configuration selected closely follows that of Turns and Myhr [1] since a large comparative data base with respect to radiation and NO_x emissions exists for these flames.

Studies have focused on soot volume fraction measurements using laser-induced incandescence (LII), OH radical and polycyclic aromatic hydrocarbon (PAH) measurements using laser-induced fluorescence (LIF) and temperature measurements using Coherent Anti-Stokes Raman Spectroscopy (CARS). The application of the LII technique for soot measurements is noteworthy since it allows quantitative soot volume fraction measurements to be obtained locally. Recent studies of the LII technique have demonstrated that it is capable of

quantitative soot volume fraction measurements if an appropriate calibration source is utilized [2-4].

Earlier reports on these current studies have noted that observed instantaneous soot volume fraction may be an order of magnitude larger than the temporally averaged mean value. This fact was attributed to the highly wrinkled structure of the turbulent flames that leads to localized high concentrations of soot particles that when temporally (and consequently spatially) averaged over the flame result in significantly lower mean values. Furthermore, the results indicated that three distinct zone soot formation/destruction regions exist. The first region is characterized by rapid soot growth in which the soot particles and OH radicals exist in distinctly separate regions of the flame. As the Reynolds number is increased, the soot particle laden region shifts towards the center of the flame. Following this region of growth, which is clearly demarcated by the absence of PAH fluorescence as indicated from the LIF-PAH imaging measurements, a mixing dominated zone is observed that is strongly affected by increases in the Reynolds number. Mixing processes in this region affect the maximum soot volume fraction measured in an individual flame with the soot volume fraction decreasing with increasing Reynolds number. The final region is characterized by an overlapping of the soot particle and OH radical fields that leads to rapid oxidation of the soot. Only the high concentration regions formed lower in the flame survive this region to be emitted from the flame as smoke.

In order to characterize spatial soot formation processes, quantitative analysis for soot volume fraction, OH radical and soot zone thickness variations, probability and integral length scales have been performed. Turbulence is shown to influence the amount of soot formed, but does not affect the characteristic profiles of the soot particle distribution in the flame. The primary effect of the turbulence is to broaden the radial soot concentration profile at a given axial position. Measurements of the soot and OH radical zone thickness show that the soot zone thickness varies linearly in the formation region, while approximately a doubling of thickness of the OH radical zone is evident over the Reynolds number range studied in these flames. Probability density functions for soot, OH radical and PAH indicate that OH radical and PAH are spatially interrelated to soot formation and oxidation processes. The shape of the probability density function for soot particles shows an exponential distribution with highly positive skewness. Based on measurements of species eddy size variations, soot and OH radical length scales show anisotropic patterns with axial preferential orientation in the streamwise direction. These measurements also indicate that the OH radical length scale is the largest and PAH is the smallest among three species at a given axial position.

More detailed information on the length scales is presented by analyzing the axial and radial variations of the eddy size of the soot volume fraction and OH radical fields. A comparison of average eddy sizes was obtained for two different Reynolds numbers, 8000 and 12,000. The average eddy size is defined as half the average integral length scale. Soot eddy size at $r/d = 0$ and $r/d = \pm 10$ as a function of the axial position is plotted in Figure 1.

The maximum soot eddy size is approximately 7 mm (~3d) with the eddy size at $r/d = 0$ increasing linearly along the jet axis for both turbulent cases. Eddies at $r/d = \pm 10$ are very asymmetric. Soot eddy size at $r/d = \pm 10$ rapidly grows until reaching the middle flame height, but this increase ceases above the middle of the flame and levels off further downstream. In particular, the effect of turbulence is more pronounced below the middle of the flame In contrast to soot eddy size, OH radical eddy size at $r/d = 0$ and $r/d = \pm 10$, surprisingly always increases along the flame as illustrated in Figure 2 even though the flame is frequently broken by air entrainment. The maximum OH radical eddy size is observed to be approximately 12 mm (~5d) for the higher Reynolds number flame.

For the soot length scales, at $r/d = \pm 10$ they are seen to increase with axial position throughout the formation region. The increase in length scale ceases in the oxidation region because parcels of air are entrained into the flame boundary and produce high intermittency in the

soot particle field and thus, breakdown the soot field structure. Moreover, oxidation due to OH radicals reduces the soot concentrations and, in turn, reduces the size of the eddies already formed. On the other hand, length scales on the axis increase with axial position throughout the flame because of the lower soot intermittency compared to the intermittency off the flame axis. In contrast to the soot, OH radical length scales at $r/d = 0$ and $r/d = \pm 10$ increase over the entire flame.

An analysis of the radial dependence of eddy sizes for the soot and OH radical fields is shown in Figure 3. Eddy sizes off the jet axis at a given axial position were ratioed by those on the jet axis. There is relatively little radial dependence with increasing Reynolds number for the soot eddy size in the oxidation regions while some variation is observed in the formation region ($y/d < 120$). The observation that the radial eddy size variation for soot particles for both turbulent cases changes little further downstream, implies that the soot eddy is moving off the axis very fast compared to the mixing rate. However, soot eddies in the formation region undergo severe turbulence flow field effects during their radial movement. With increasing Reynolds number, a weak radial dependence of soot eddy size can be observed. However, a difference exists in the OH radical case such that OH radical eddy sizes off the axis are always larger than those on the axis except near the flame tip. There is a remarkably radial uniformity compared to the average and fluctuations of soot that show large radial dependencies. These radial variations arise from the intermittency of the soot field. As pointed out by Dasch et al. [5], the radial uniformity of soot eddies implies that the soot chemistry in the soot-containing regions is relatively slow compared to the radial mixing.

From the CARS temperature measurement, single-shot temperature spectra obtained show fairly good agreements with theoretical N_2 spectra. A method to obtain the fuel diffusion layer in which average stoichiometric conditions are locally satisfied is suggested by analyzing the correlation between temperature and unburned fuel. In the temperature pdfs, temperature bimodality is observed over all the axial positions and the bimodality width with respect to radial distance increases with increasing Reynolds number. With respect to soot formation, the highest soot formation and the peak mean temperature are observed on the fuel-rich side of the stoichiometric flame location while the peak OH· concentration lies on the fuel-lean side.

REFERENCES

1 Turns, S. R. and Myhr, F. H., "Oxides of Nitrogen Emissions from Turbulent Jet Flames Part I – Fuel Effects and Flame Radiation," *Combustion and Flame*, 87:319-335, 1991.

2 Quay, B., Lee, T-W, Ni, T. and Santoro, R. J., "Spatially Resolved Measurements of Soot Volume Fraction Using Laser-Induced Incandescence," *Combustion and Flame*, 97:384-392, 1994.

3 Ni, T., Pinson, J. A., Gupta, S. and Santoro, R. J., "Two-Dimensional Imaging of Soot Volume Fraction by the Use of Laser-Induced Incandescence," *Applied Optics*, 34, pp. 7083-7091, 1995.

4 Ni, T., Gupta, S., and Santoro, R. J., "Suppression Of Soot Formation In Ethene Laminar Diffusion Flames By Chemical Additives," *Twenty-fifth Symposium (International) on Combustion,* The Combustion Institute, 1994, pp. 585-592.

5 Dasch, C. J. and Heffelfinger, D. M., "Planar Imaging of Soot Formation In Turbulent Ethylene Diffusion: Fluctuations and Integral Scales," *Combustion and Flame*, 85:389-402, 1991.

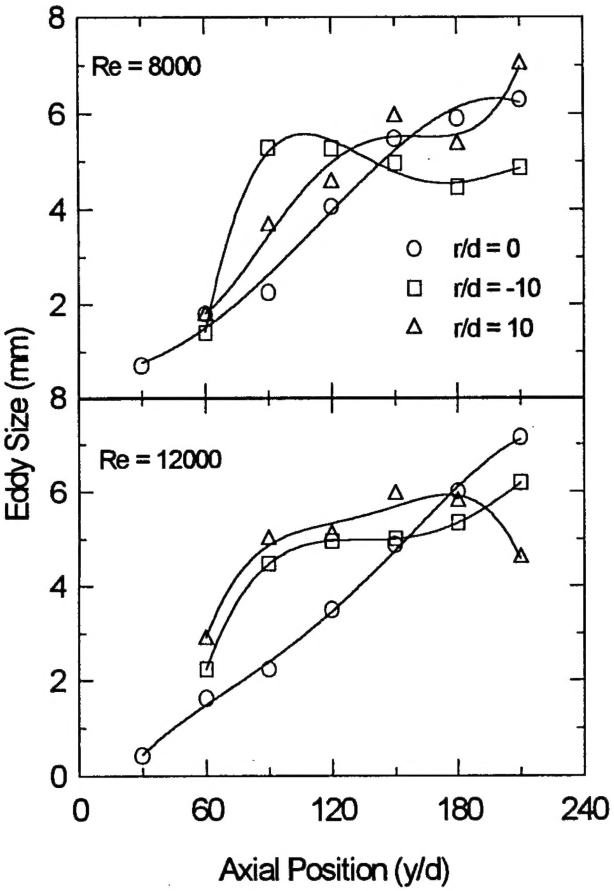

Figure 1. Average soot eddy size as a function of axial position for Re = 8000 and 12000 flames

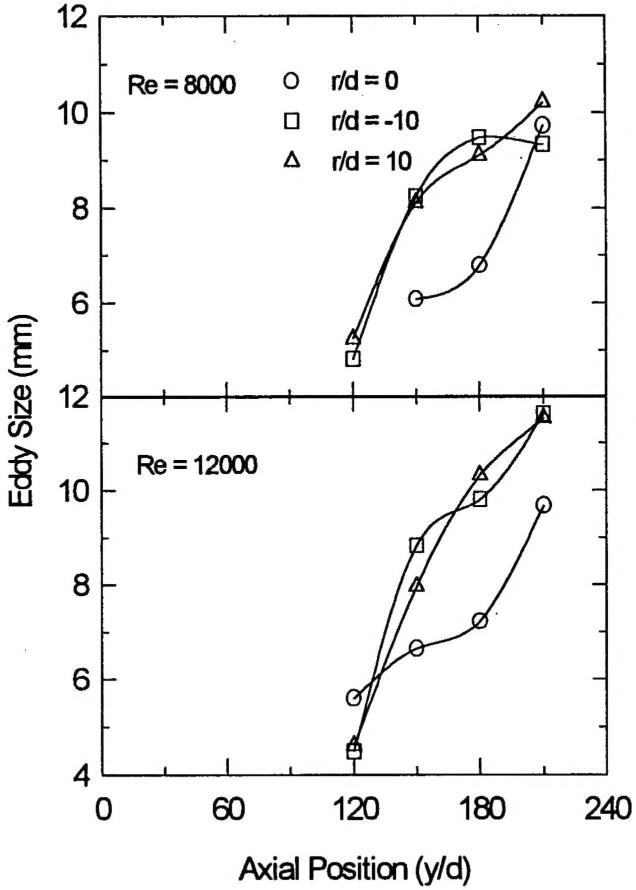

Figure 2. Average OH• eddy size as a function of axial position for Re = 8000 and 12000 flames

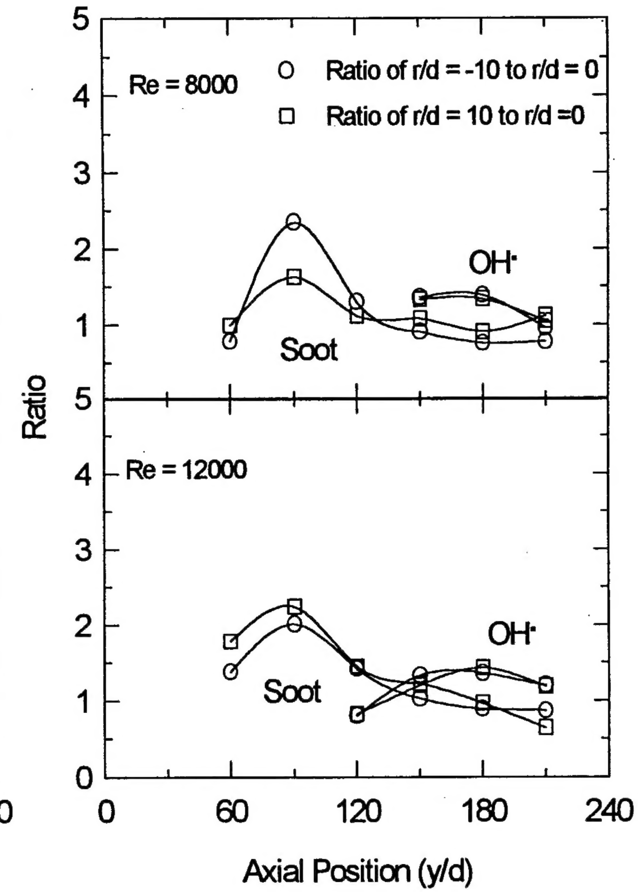

Figure 3. Radial variation of the soot particle and OH• eddy size for Re = 8000 and 12000 flames

Personnel Supported

Dr. Robert J. Santoro	Principal investigator
Mr. Seong-Young Lee	Graduate Student Research Assistant
Mr. Larry Horner	Technician

Publications

Peer-reviewed publications
None

Book Chapters Published
None

Interactions/Transitions

a. Participation/presentations at meetings, conferences, etc.

Broda, J. C., Santoro, R. J., Shirhattikar, G., and Yang, V., "An Experimental Study of Combustion Dynamics in a Premixed Swirl Injector," The Twenty-Seventh International Symposium on Combustion, University of Colorado at Boulder, August 2-7, 1998.

Rapp, D. C. and Santoro, R. J., "Species Measurements in Coannular, Laminar Diffusion Flames," The Twenty-Seventh International Symposium on Combustion, University of Colorado at Boulder, August 2-7, 1998.

Lee, S-Y. and Santoro, R. J., "Imaging Studies of Soot Formation in Turbulent Ethylene Jet Flames," The Eastern States Fall Technical Meeting, Hartford, CT, October 27-29, 1997.

Rapp, D. C. and Santoro, R. J., "Analysis of Soot Particle Inception in a C_2H_4/Air, Coannular, Laminar Diffusion Flame," The Eastern States Fall Technical Meeting, Hartford, CT, October 27-29, 1997.

Lee, S-Y., Pal, S. and Santoro, R. J., "Temperature and Unmixed Fuel Measurements in Turbulent Jet Flames by Using Coherent Anti-Stokes Raman Spectroscopy," The Eastern States Fall Technical Meeting, Hartford, CT, October 27-29, 1997.

Broda, J.C., Seo, S., Pal, S. and Santoro, R. J., "Recent Experimental Results in High Pressure Gas Turbine Combustion Instabilities," The Eastern States Fall Technical Meeting, Hartford, CT, October 27-29, 1997.

b. Consultant and advisory functions to other laboratory and agencies, especially Air Force and other DoD laboratories

Member NASA Combustion Science Discipline Working Group, NASA.

Advisor to Air Force Research Laboratory, Aeropropulsion and Power Directorate, on combustion instability phenomena.

Short Course: "Introduction To Pulse Detonation Engines", Presented at the Air Force Research Laboratory, Wright-Patterson Air Force Base, May 12 and 13, 1998 (with J. C. Broda and V. Yang)

Reviewer For the Department of Energy, Office of Basic Energy Sciences, for the Combustion Research Facility at Sandia National Laboratories, Livermore, CA, March 9-11, 1998.

Panelist for the "Second AGARD Workshop on Active Combustion Control for Propulsion Systems," The Von Karman Institute Brussels, Belgium, October 16-18, 1997.

c. Transitions

1. Provided data on soot, velocity, species, and temperature fields in laminar diffusion flames to Exxon Research and Engineering Company for use in development and validation of instrumentation for measuring soot and temperature fields.
Contact:
Dr. Jeffrey M. Grenda
Exxon Research and Engineering Company
Route 22 E. Clinton Township
Annandale, NJ 08801
Tel: (908) 730-2545
Fax: (908) 730-3198
E-mail: jmgrend@erenj.com

2. Transferred expertise in laser-induced incandescence technique for smoke measurements in rocket plumes to MetroLaser, Inc. This information was utilized to develop non intrusive optical diagnostic approach for measurements in rocket exhaust plumes for health monitoring.
Contact:
Dr. Serdar Yeralan
MetroLaser, Inc.
18010 Skypark Circle,
Suite 100
Irvine, CA 92614
Tel: (949) 553-0688
Fax: (949) 553-0495
E-mail: syeralan@metrolaserinc.com

New discoveries, inventions or patent disclosures

None

Honors/Awards

None

Table 1. 1998 BASIC RESEARCH TECHNOLOGY TRANSITIONS

(Grant: F49620-97-1-0094, P. I.: R. Santoro)

	Performer	**Customer**	**Result**	**Application**
1	R. J. Santoro Penn State University (814) 863-1285	Dr. Jeffrey M. Grenda Exxon Research and Engineering Company, Route 22, Clinton Township Annandale, NJ 08801 (908) 730-2545	Provided data on soot, velocity, species and temperature fields in laminar flames for use in development and validation of instrumentation for measuring soot and temperature fields.	Instrumentation development for commercial combustion devices (furnaces, gas turbines, etc.)
2	R. J. Santoro Penn State University (814) 863-1285	Dr. Serdar Yeralan MetroLaser, Inc. 18010 Skypark Circle, Suite 100 Irvine, CA 92614 (949) 553-0688	Transfer of expertise in laser-induced incandescence technique for smoke measurements in rocket plumes.	Non intrusive optical diagnostic instrumentation development for smoke measurements in rocket exhaust plumes for health monitoring.

Principal Investigator Annual Data Collection (PIADC) Survey Form

NOTE: If there is insufficient space on this survey to meet your data submissions, please submit additional data in the same format as identified below.

PI DATA

Name (Last, First, MI) Santoro, Robert, J.

Institution The Pennsylvania State University

Contract/Grant No. F49620-97-1-0094

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Project/Subarea
____ / ____

NX ____________

FX ____________

NUMBER OF CONTRACT/GRANT CO-INVESTIGATORS

Faculty 1   Post Doctorates 0   Graduate Students 1   Other 0

PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

NOTE List names in the following format: Last Name, First Name, MI

Include Articles in peer reviewed publications, journals, book chapters, and editorships of books.

Do not include Unreviewed proceedings and reports, abstracts. "Scientific American" type articles, or articles that are not primary reports of new data and articles submitted or accepted for publication, but with publication date outside of the stated time frame.

Name of Journal, Book, etc. **None**

Title of Article ____________

Author(s) ____________

Publisher (if applicable) ____________

Volume: ______ Pages: ____ Month Published: ______ Year Published: ______

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Include: All honors and awards received during the lifetime of the contract or grant, and any lifetime achievement honors such as (Nobel prize, honorary doctorates, and society fellowships) prior to this contract or grant.

Do Not Include: Honors and awards unrelated to the scientific field covered by the contract/grant.

Honor/Award: **None**   Year Received: ______

Honor/Award Recipient(s): ____________

Awarding Organization: